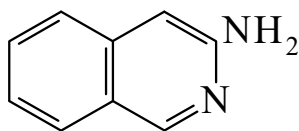




>>Entry Name: 3-Aminoisoquinoline

Synonym(s): 3-Isoquinolinamine, 9CI



CAS Registry Number: 25475-67-6

Molecular Formula: C₉H₈N₂

Molecular Weight: 144.176

Accurate Mass: 144.068748

Percentage Composition: C 74.98%; H 5.59%; N 19.43%

Physical Description: Yellow solid (C₆H₆)

Melting Point: Mp 178°

pKa Value: pK_a 5.03 (20°)

Rare Chemicals Library: S90926-2

>>Derivative: *N*-Me

Synonym(s): 3-Methylaminoisoquinoline

CAS Registry Number: 171861-48-6

Molecular Formula: C₁₀H₁₀N₂

Molecular Weight: 158.202

Accurate Mass: 158.084398

Percentage Composition: C 75.92%; H 6.37%; N 17.71%

Physical Description: Cryst. (C₆H₆/hexane)

Melting Point: Mp 87-89°

>>Derivative: *N,N*-Di-Me

Synonym(s): 3-Demethylaminoisoquinoline

CAS Registry Number: 171861-54-4

Molecular Formula: C₁₁H₁₂N₂

Molecular Weight: 172.229

Accurate Mass: 172.100048

Percentage Composition: C 76.71%; H 7.02%; N 16.27%

Melting Point: Mp 35-36°

>>Derivative: *N-tert*-Butyl

CAS Registry Number: 171861-49-7

Molecular Formula: C₁₃H₁₆N₂

Molecular Weight: 200.283

Accurate Mass: 200.131348

Percentage Composition: C 77.96%; H 8.05%; N 13.99%

Boiling Point: Bp_{0.01} 95°

>>Derivative: *N*-Ph

Synonym(s): 3-Anilinoisoquinoline

CAS Registry Number: 171861-52-2

Molecular Formula: C₁₅H₁₂N₂

Molecular Weight: 220.273

Accurate Mass: 220.100048

Percentage Composition: C 81.79%; H 5.49%; N 12.72%

Melting Point: Mp 103-105°

References:

Teague, C.E. *et al.*, *J.A.C.S.*, 1951, **73**, 688-689, (*synth*)

Johnson, F. *et al.*, *J.O.C.*, 1962, **27**, 3953-3958, (*synth*)

Zdrojewski, T. *et al.*, *Tetrahedron*, 1995, **51**, 12439-12444, (*synth*, *pmr*, *cmr*, *derivs*)